

On the identity of the radiation-induced stable alanine radicalEwald Pauwels^{1*}, Hendrik De Cooman¹, Michel Waroquier¹, Eli O. Hole², Einar Sagstuen²¹Center for Molecular Modeling, Ghent University, Technologiepark 903, B-9052 Zwijnaarde, Belgium

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Supporting Information

Table SI-1

Isotropic and anisotropic hyperfine couplings (in MHz) and g-tensor values of the stable alanine radical (experiment) and two model structures. The last column indicates the angle (in degrees) between corresponding experimental and calculated eigenvector directions.

		$A_{\text{iso}}/g_{\text{iso}}$	$A_{\text{aniso}}/g_{\text{aniso}}$	Angle
Experiment	H_{β}	69.9	-2.6	
			-2.3	
			4.8	
	H_{α}	-56.1	-31.8	ref ²
			3.9	
			27.9	
	g	2.0033	2.0024	
			2.0034	
			2.0041	
	$H(\text{N})$	0.2	-4.0	ref ⁴
-1.7				
5.7				
B-1	H_{β}	17.8	-2.4	60
			-1.7	68
			4.1	34
	H_{α}	-20.6	-14.9	86
			-3.0	87
			17.9	28
	g	2.0035	2.0022	39
			2.0037	33
			2.0046	27
	$H(\text{N})$	4.3	-3.6	87
-2.9			83	
6.5			36	
B-2	H_{β}	23.3	-2.4	59
			-1.7	63
			4.1	35
	H_{α}	-21.6	-17.6	90
			-3.2	85
			20.8	27

		2.0022	55
g	2.0036	2.0039	59
		2.0048	26
		-4.2	78
H(N)	-2.2	-1.0	51
		5.2	80

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